Overview of Modeling and Simulation

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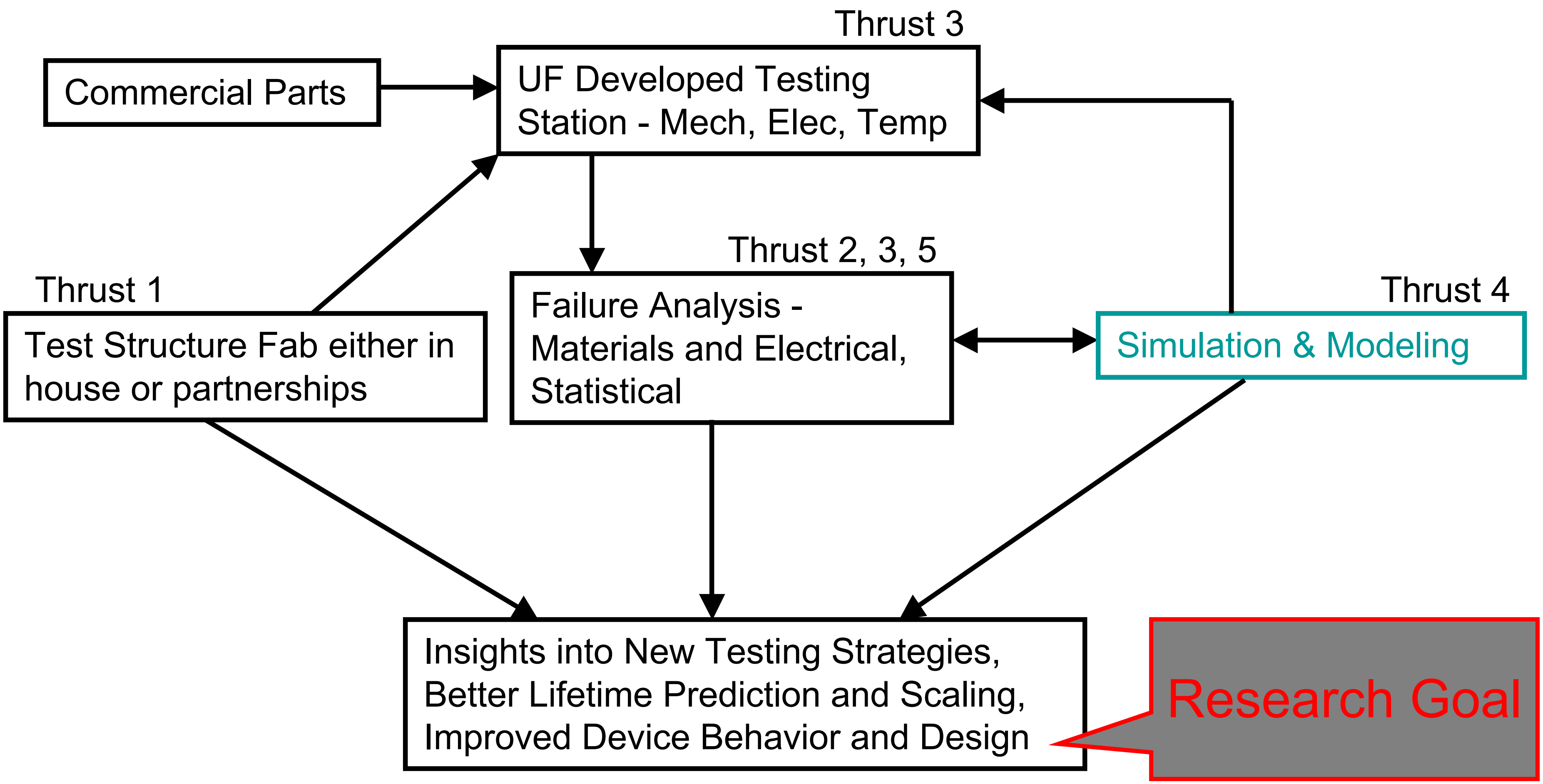
Outline

- Modeling Overview
- Device Simulation Development
- Strain Effects
- Temperature
- Trapping
- Directions

Research Work Plan



Lifetime Prediction

Roesch, 2006

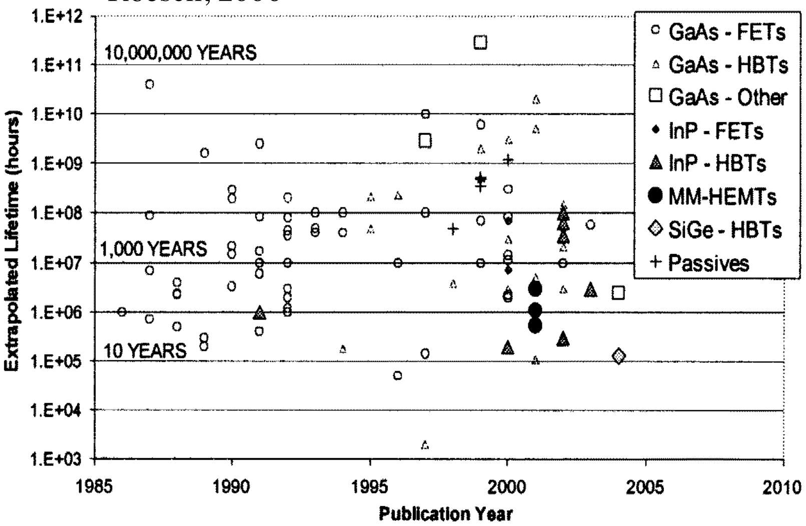
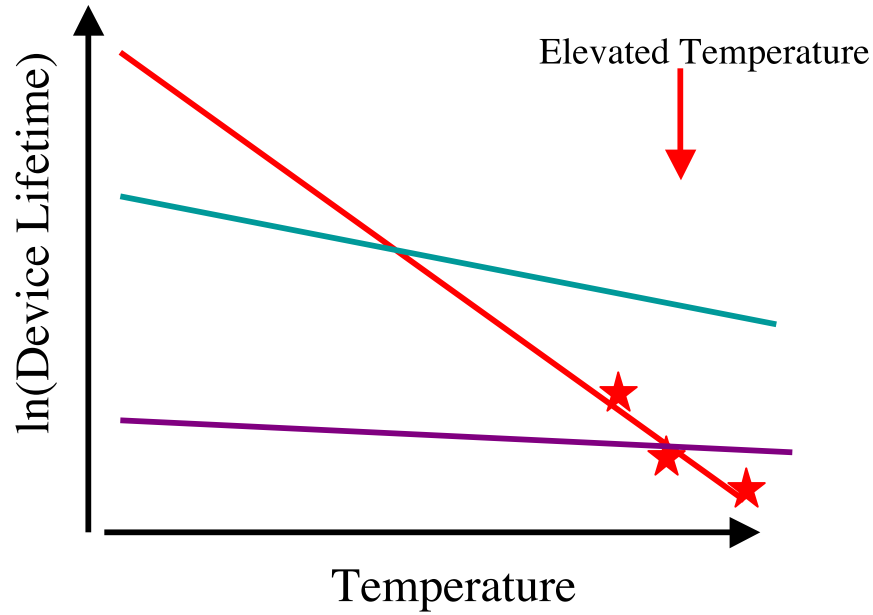


FIGURE 1. REPORTED OPERATING LIFETIMES FOR VARIOUS COMPOUND SEMICONDUCTORS OVER THE 19 YEAR HISTORY OF THE ROCS WORKSHOP[1]



- Project Life Time
- Temperature Acceleration Approach
- Modeling is critical in extrapolation

FLOOPS / FLOODS / FLOORS

- Object-oriented codes
- Multi-dimensional
- P = Process / D = Device 90% code shared
- Scripting capability for PDE's - Alagator

- Commercialized - ISE / Synopsis
  - Sentaurus - Process is based on FLOOPS
- Licensed at over 400 sites world-wide
  - 2008 release
  - Manual is online (building a wiki manual)

What is Alagator?

- Scripting language for PDE's
- Parsed into an expression tree
- Assembled using FV / FE techniques
- Stored in hierarchical parameter data base

- Models are accessible, easily modified

What is Alagator?

Operator	***Description***
“ddt”	Time derivative
“grad”	Spatial derivative
“sgrad”	Scharfetter / Gummel Discretization Operator
“dot”	Returns the dot product of the gradient of two field – electric field in direction of current flow
“elastic”	Compute elastic forces - FEM balance

- Example use of operators for diffusion equation
- Fick’s Second Law of Diffusion
  - ddt(Boron) - 9.0e-16 * grad(Boron) - K * (Boron - Trap)
  - $\partial C(x,t) / \partial t = D \partial^2 C(x,t) / \partial x^2 - K * C(x,t) * C_T$

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Discretization – PDE's

- The set of coupled, time-dependent partial differential equations that govern semiconductor device behavior can be written as

$$\nabla \cdot (\varepsilon \nabla \psi) = -q\left(p - n + N_D^+ - N_A^-\right)$$

1. Poisson Equation

$$\frac{dn}{dt} = \frac{1}{q}\nabla \cdot J_n - U_n$$

2. Electron Continuity Equation

$$\frac{dp}{dt} = -\frac{1}{q}\nabla \cdot J_p - U_p$$

3. Hole Continuity Equation

ε - dielectric permittivity
ψ - electrostatic potential
n, *p* - electron, hole densities
J_n, J_p – electron, hole current densities
U_p, U_n - net recombination rates
N_D^+, N_A^- - ionized donor and acceptor densities

Discretization – Current Density

Quasi-Fermi Current Density

$$J_n = -q\mu_n n \nabla \phi_n$$

$$J_p = -q\mu_p p \nabla \phi_p$$

Boltzmann Relations

$$\phi_n \equiv \psi - \frac{kT}{q}\ln\left(n / n_i\right)$$

$$\phi_p \equiv \psi + \frac{kT}{q}\ln\left(p / n_i\right)$$

Drift-Diffusion Current Density

$$J_n = qn\mu_n \mathrm{E} + qD_n \nabla n$$

$$J_p = qp\mu_p \mathrm{E} - qD_p \nabla p$$

- To obtain a closed system of equations, current densities written as function quasi-Fermi levels
- Using Boltzmann relations, current density can be written in the familiar relationship as the sum of drift and diffusion components

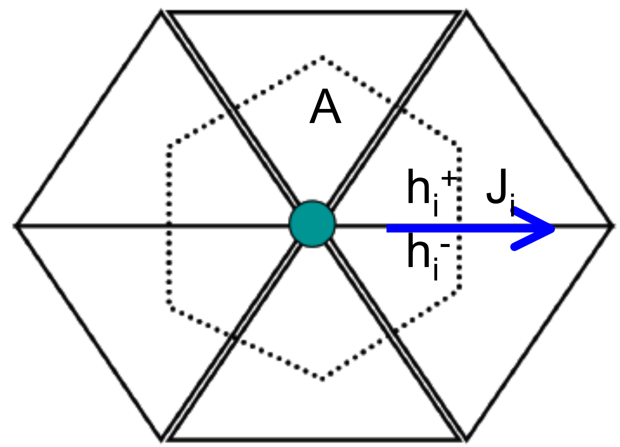
- Drift-Diffusion subtracting large numbers is not a good recipe with finite precision arithmetic

Finite Volume Scharfetter-Gummel (FVSG)

- Each PDE is integrated over a control volume *A*
- A is defined by the perpendicular bisectors of mesh elements
- PDe integrated using Green's formula
- Current $J_{n,p}$ evaluated using the Scharfetter-Gummel
- Scharfetter Gummel
  - Assume field and current constant
  - Solve resulting equation
  - $J_n/q = D\ (\ B(t)\ n_i+ - B(-t)\ n_i-\ )\ /\ l_i$
  - $t = \mu\ E\ /\ D$
  - $B(t) = t\ /\ (e^t - 1)$ Bernoulli Function

$$J_n = qn\mu_n \mathrm{E} + qD_n \nabla n$$

$$\frac{dn}{dt} = \frac{1}{q}\nabla \cdot J_n - U_n$$



$$\frac{1}{q}\sum_i J_i\left(h_i^+ + h_i^-\right) - A\left(U_n + \frac{dn}{dt}\right) = 0$$

- Advantages:
  - Commonly used "proven" method
  - Assembly time, each edge assembled once
- Disadvantages
  - Current defined only on edges, not continuous in space
  - Impact Ionization, Joule Heating more difficult
  - Works best when grid is aligned with current flow

Finite Element Quasi-Fermi (FEQF)

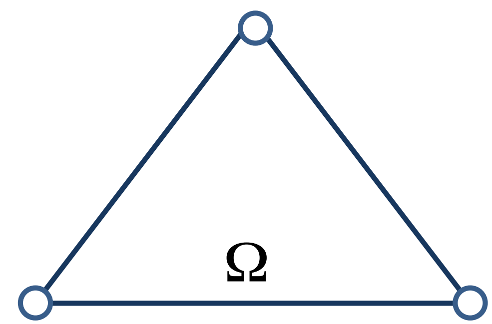
- $\phi_{n,p}$ defined at grid nodes
- Use shape function in an element
  - Piecewise linear most common
  - Can be higher order
- Integrate equations and minimize error

- Advantages:
  - Current is a continuous function over each element
  - Easier to compute Joule Heating, Impact Ionization
  - Compatible with strain calculations

- Disadvantages
  - Not as stable
  - Convergence issues

$$J_n = -q\mu_n n \nabla \varphi_n$$

$$\frac{dn}{dt} = \frac{1}{q} \nabla \cdot J_n - U_n$$



$$a(\psi, v) \equiv (-\rho, v)$$

$$a(\psi, v) \equiv \iint_{\Omega} \varepsilon \nabla \psi \cdot \nabla v \, dx \, dy$$

$$(-\rho, v) \equiv -\iint_{\Omega} \rho \, v \, dx \, dy$$

FLOODS - Numerical Approximations

Nonlinear set of PDE

Poisson
Carrier Continuity

↓ Temporal and Spatial Discretization

Nonlinear algebraic equations

Flux = $(n_1 - n_2) / x_{12}$

↓ Multi-dimensional Newton Linearization

Linear Matrix Problem

$$\frac{1}{x_{12}}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \cdot \begin{bmatrix} \Delta n_1 \\ \Delta n_2 \end{bmatrix} = \begin{bmatrix} F \\ F \end{bmatrix}$$

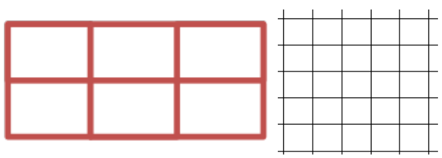
- Discretization
  - Replace continuous functions w/ piecewise linear approximations
  - Grid Spacing, Time
- Linearization
  - Reduce nonlinear terms using multi-dimension Newton’s method
- Linear Matrix Problem
  - Number of PDE’s x number of nodes square
  - Direct Solver (UMFPACK)
- Assembly of Matrix
  - Calculate the large, linear system
  - Linear in number of elements
- Solution of Matrix
  - Large Sparse System
  - Low power of equations $n^{1.5}$

Mesh Elements

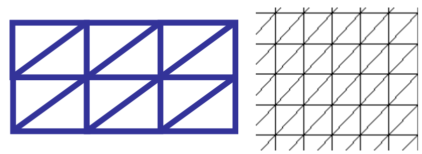
- Both FVSG and FEQF methods were compared for a variety of mesh element types and device structures.
- The follow elements were tested using the different discretization methods:

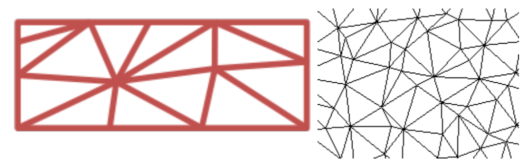
2-D:

Quad



Quad-Diagonal

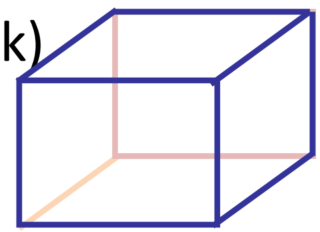




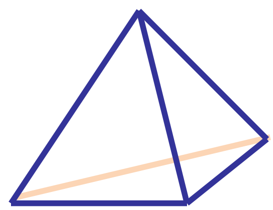
non-rectilinear

3-D:

Hexahedron (Brick)



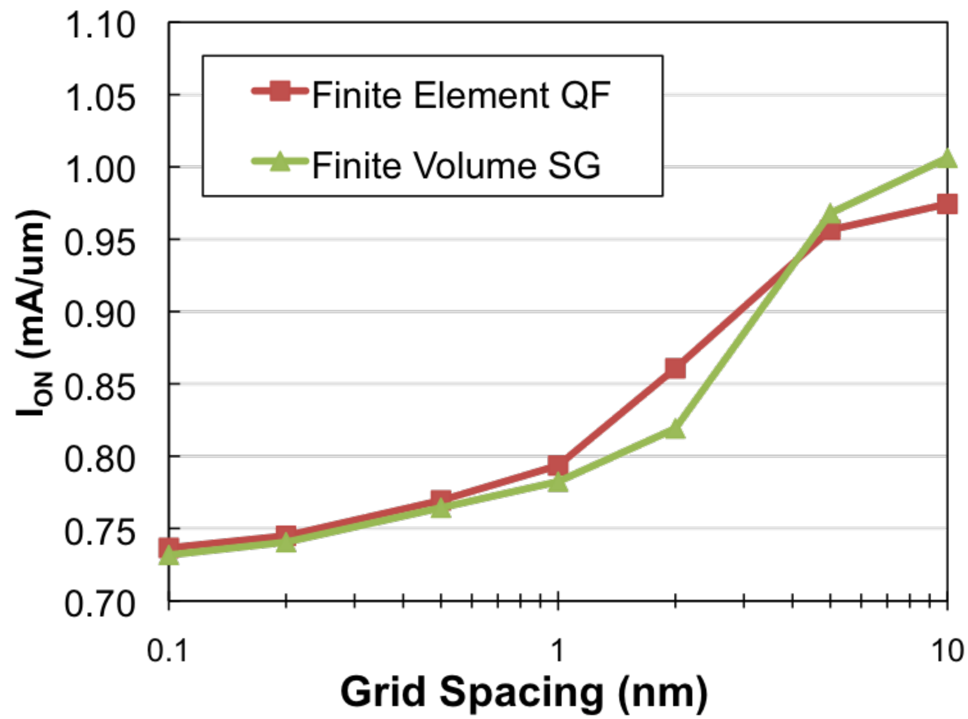
Tetrahedron



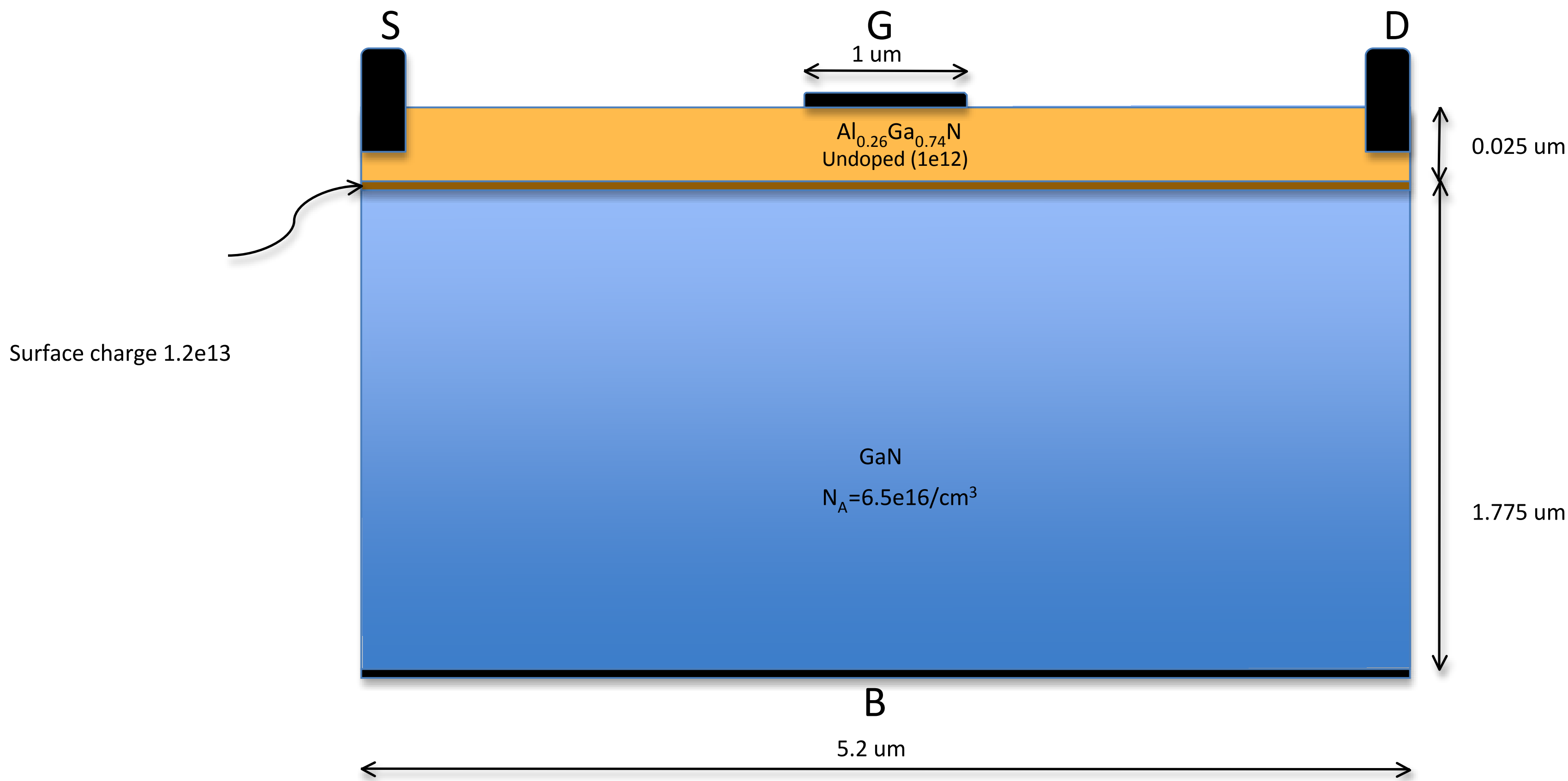
- The x-, y-, z-axis grid spacings were varied
  - Accuracy vs. computation time

MOSFET – Discretization Error

- For nMOS, FVSG and FEQF methods gave agreeing results
  - Quad & Quad-diagonal
  - Output current
- As grid spacing increases, discretization error is introduced resulting a overestimated current output



HEMT Structure



[Not to scale]

Mobility Model

Future work on strain-induced polarization demands a robust mobility model which includes field dependence

- Farahmand, et. al., IEEE Trans. Elec. Dev., 48, no. 3, 2001
  - Low-field mobility
    - Drift-diffusion
      - Influence of temp (T) and ionized impurit concentration (N)
      - μ_{max}, μ_{min}, α, $\beta_{1\text{-}4}$
        - Parameters from Farahmand

$$\mu_0(T, N) = \mu_{\min}\left(\frac{T}{300}\right)^{\beta_1} + \frac{(\mu_{\max} - \mu_{\min})\left(\frac{T}{300}\right)^{\beta_2}}{1 + \left[\frac{N}{N_{ref}\left(\frac{T}{300}\right)^{\beta_3}}\right]^{\alpha(T/300)^{\beta_4}}}.$$

  - High-field mobility
    - Low-field + field dependent mobility
      - E: Electric field
      - E_c, v_{sat}, a, n_1, n_2
        - Parameters from Farahmand

$$\mu = \frac{\mu_0(T, N) + v^{sat}\frac{E^{n1-1}}{E_c^{n_1}}}{1 + a\left(\frac{E}{E_c}\right)^{n_2} + \left(\frac{E}{E_c}\right)^{n_1}}$$

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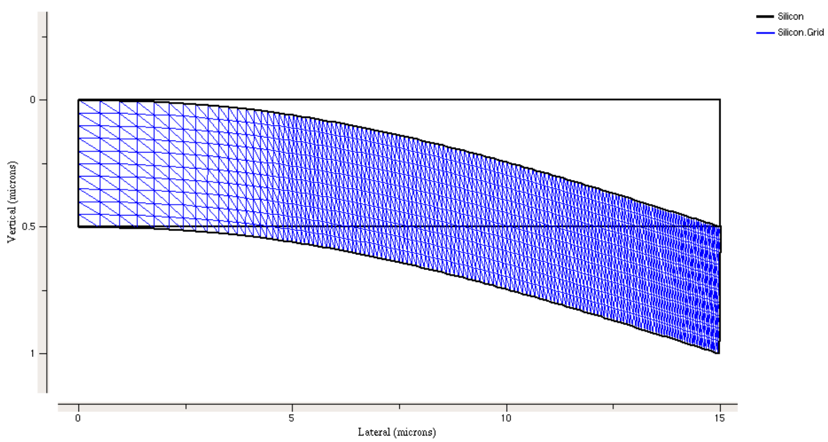
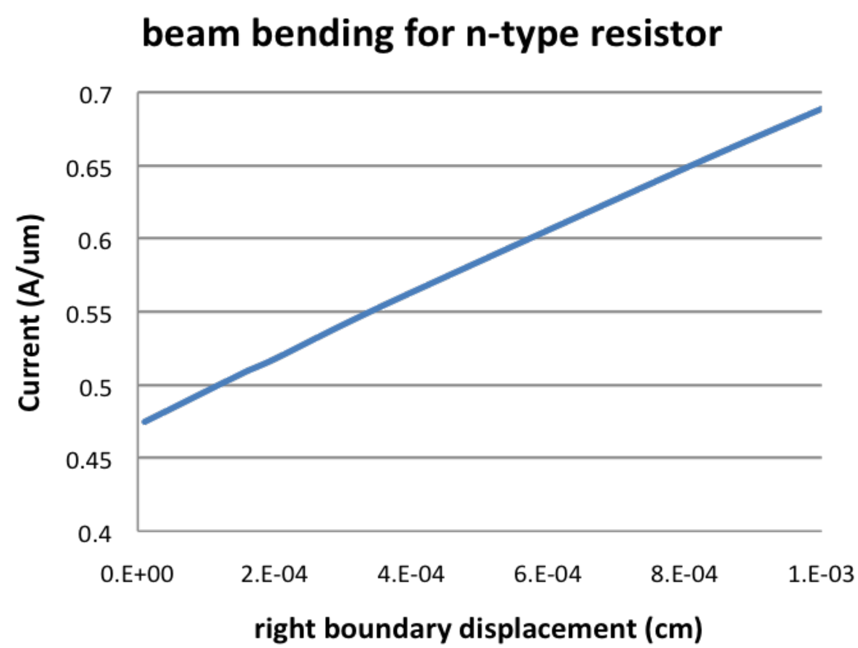
Piezoresistance example

- Silicon beam with an n-type surface
- Bending induces tensile stress at the surface resulting in a increase in mobility and current.

$$J_X(\sigma) \cong \left(1 + \frac{-\Delta\mu_{xx}}{\mu_{xx}}\right) J_X(0) = \left(1 + \pi_{11}\sigma_{xx}\right) J_X(0)$$

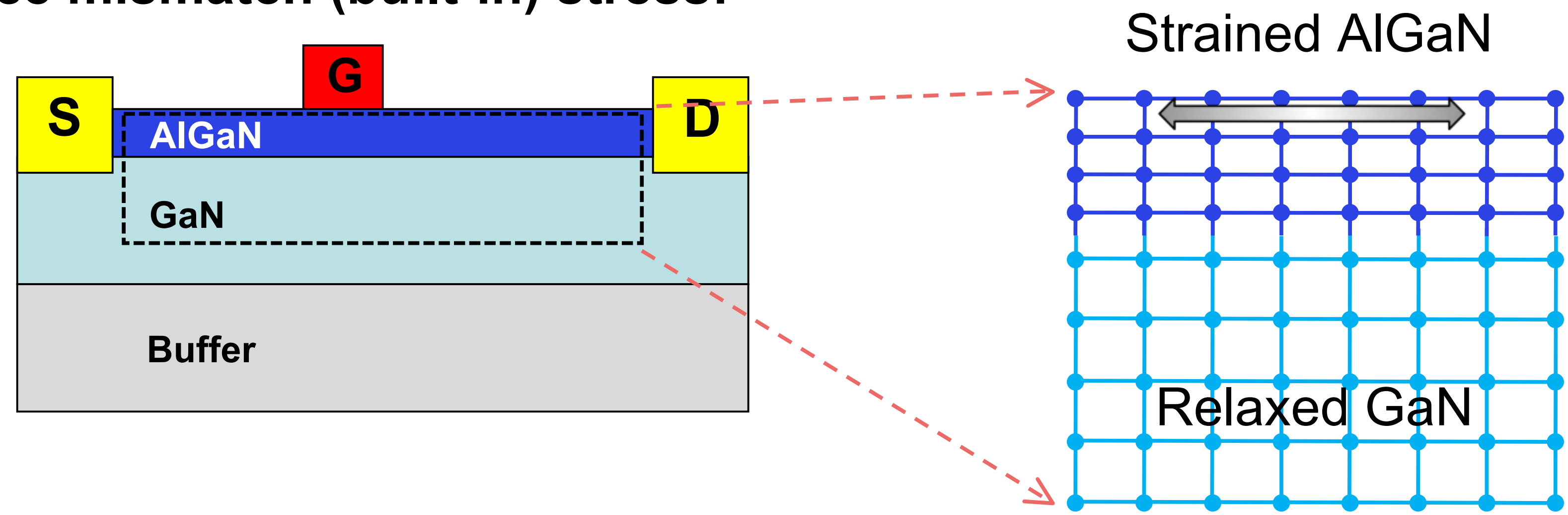


FLOOXS beam bending example

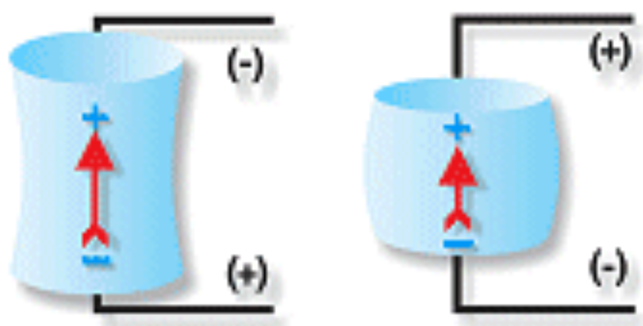


Stress in GaN HEMT Devices

Lattice mismatch (built-in) stress:



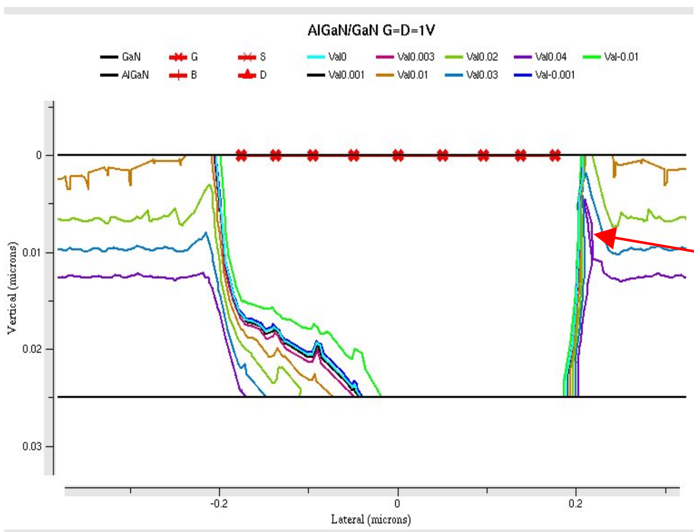
Inverse piezoelectric (generated) stress:

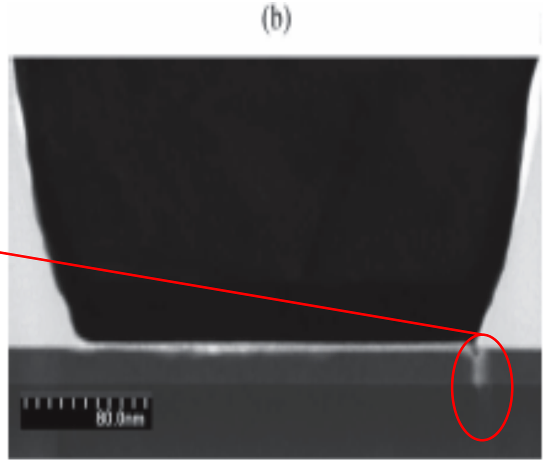


$$\begin{pmatrix} P_x \\ P_y \\ P_z \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & e_{15} & 0 \\ 0 & 0 & 0 & e_{15} & 0 & 0 \\ e_{31} & e_{31} & e_{33} & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{zx} \\ \varepsilon_{xy} \end{pmatrix}$$

Inverse Piezoelectric Effect Calculation

- Mechanical Simulation with InversePiezo and Lattice Mismatch Terms
- Low voltage applied
- Sharp bunching of strain from inversepizeo terms near drain edge

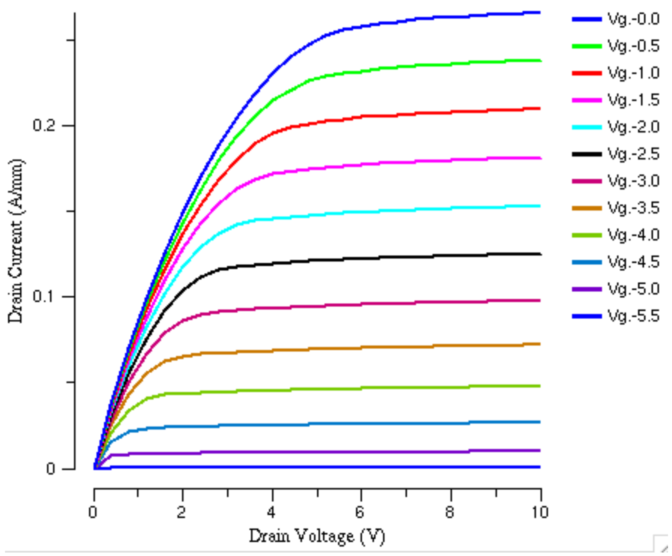




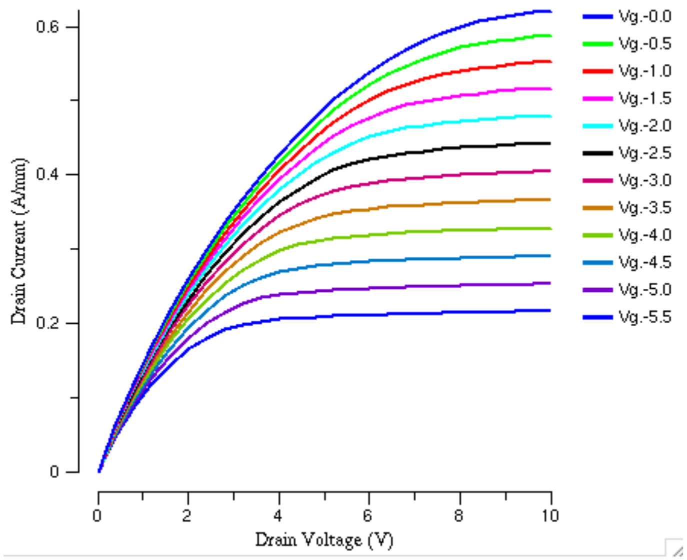
David Horton, Poster

A 21st Century Approach to Reliability

Interface Charge Effect



Interface charge 1.2e13



Interface charge 2.0e13

- Link to strain calculations
- Does change in strain change 2DEG charge?

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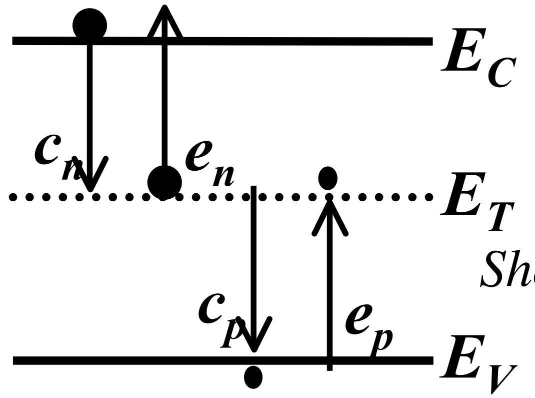
Modeling of defects



Shockley-Read-Hall Model

- Random carrier transitions between continuum states (E_C, E_V) and localized defect states.

Four basic equations with one trap level added, 3+N with N trap levels:

$$F_\psi = -\frac{d^2\psi}{dr^2} - \frac{q}{\varepsilon}\left[p - n + N_D^+ - N_A^- - n_t\right] = 0$$

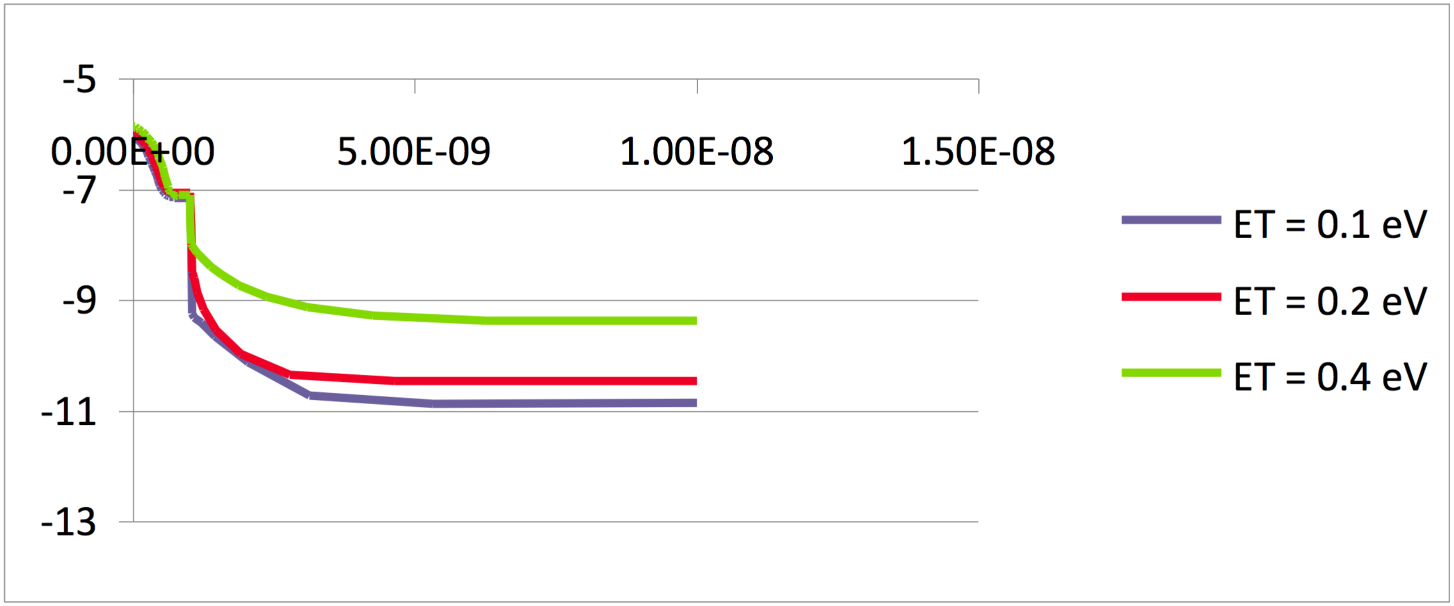
$$F_n = \frac{dn}{dt} - \frac{1}{q}\nabla \cdot \boldsymbol{J}_n - g_n + r_n - \gamma_n(\boldsymbol{r},t) = 0$$

$$F_p = \frac{dp}{dt} + \frac{1}{q}\nabla \cdot \boldsymbol{J}_p - g_p + r_p + \gamma_p(\boldsymbol{r},t) = 0$$

$$F_{n_t} = \frac{dn_t}{dt} + g_n - r_n - g_p + r_p - \gamma_t(\boldsymbol{r},t) = 0$$

Transient Trapping Results

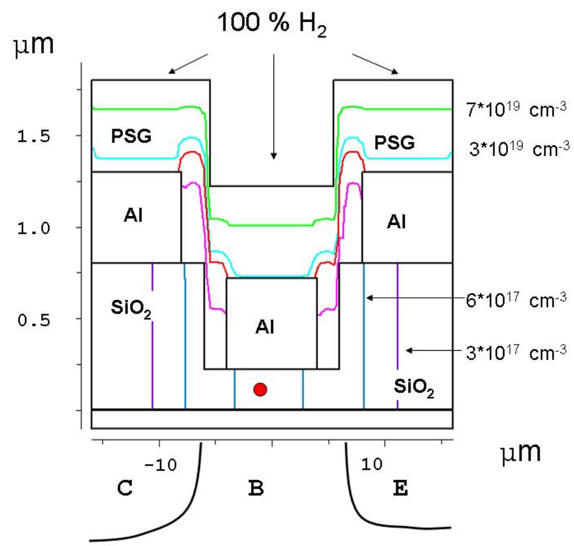
- Added slow filling traps
- I_{DS} dependence on trap level in reverse bias gate step
- Change in response time and DC level



Hydrogen Trapping Simulation

TNS, TBP
Vanderbilt + UF

- Simulate Device in Quasi-Steady State
  - Electrons and Holes equilibrate quickly
  - Similar to assumption in process simulation
- Generation Events Triggered by
  - Mechanical Stress
  - Current Flow / Electric Field
- Simultaneous solutions
  - Point Defects / Defect Cluster / Interface Capture
  - Hydrogen



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Temperature Models

All temperature dependence has been implemented

Thermal transport equations (Wachutka, IEEE Trans. Comp. Aided Des., **9**, no. 11, 1990)

$$c \cdot (\partial T/\partial t) = \text{div}\,(\kappa \vec{\nabla} T) + H$$

$\varkappa \equiv$ thermal conductivity

$c \equiv$ lattice heat capacity

	GaN	AlGaN
$\varkappa$ (W/cm•°K)	2.67	0.33
c (J/°K•cm3)	1.395	1.395

H = Heat Generation rate, several interpretations are in the literature

$$H = q \cdot \text{div}\,(\phi_n \vec{j}_n - \phi_p \vec{j}_p).$$

ϕ_n ,ϕ_p≡quasi-fermi levels of e, h

because hole concentration is negligible, simplified to

$$\vec{j}_n = \mu_n \cdot n \cdot \vec{\nabla}\phi_n$$

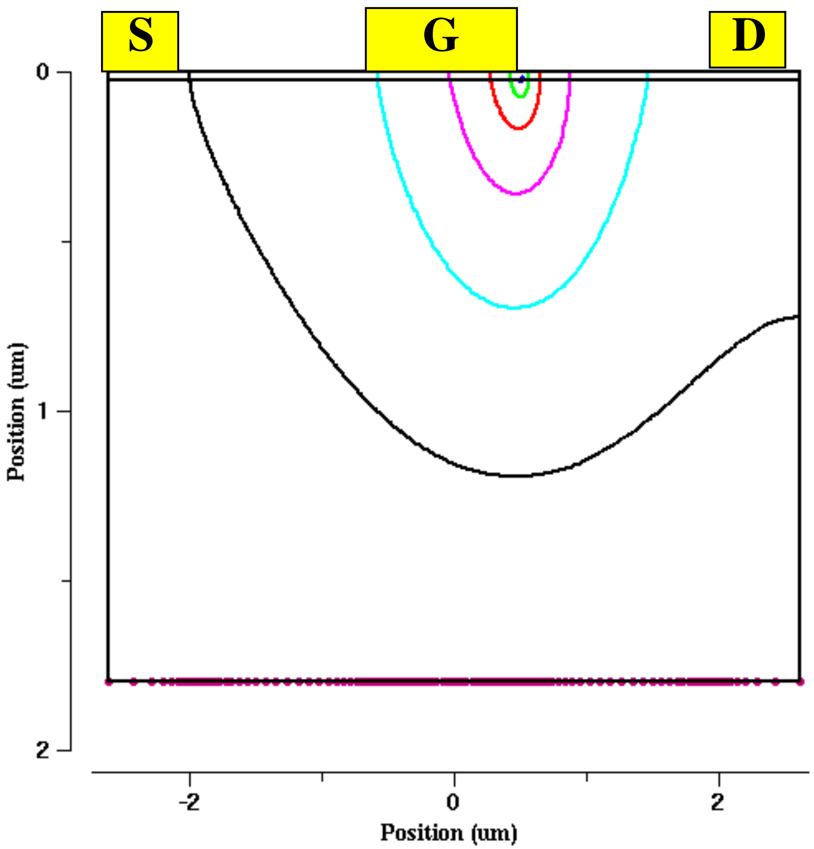
$$H = q \cdot \text{div}\,(\phi_n \vec{j}_n - \phi_p \vec{j}_p).$$

$$\vec{j}_p = -\mu_p \cdot p \cdot \vec{\nabla}\phi_p$$

Fixed temperature boundary condition applied to bulk contact:

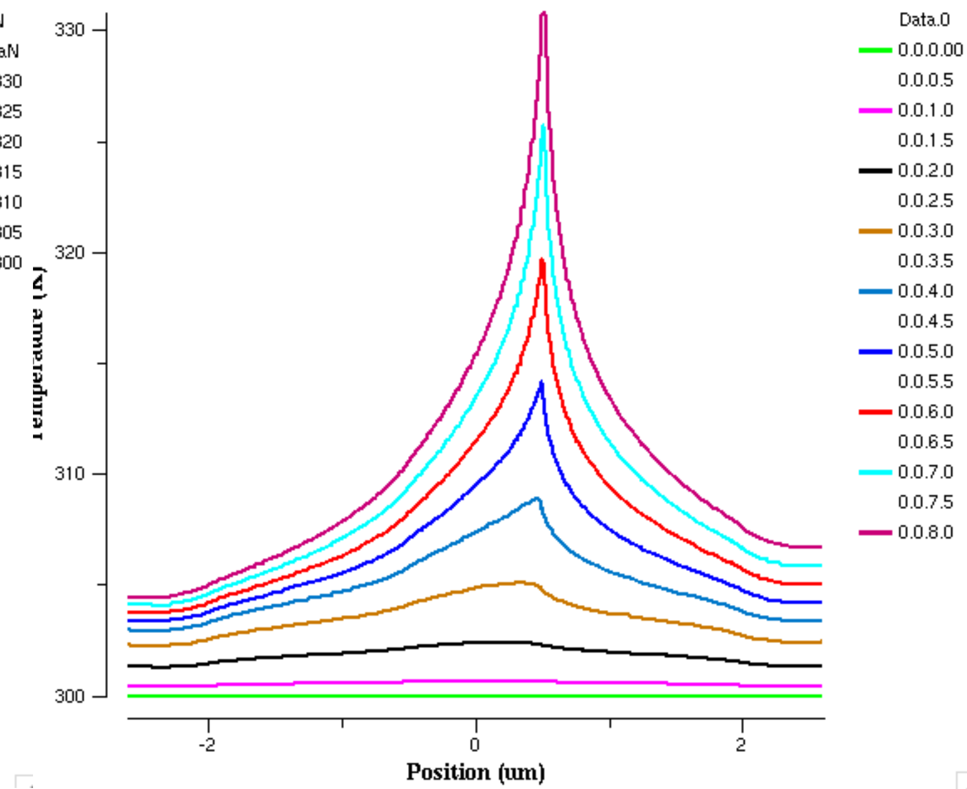
$T_{bulk\_contact}$=300 (K)

Temperature Profiles



Contour plot of temperature

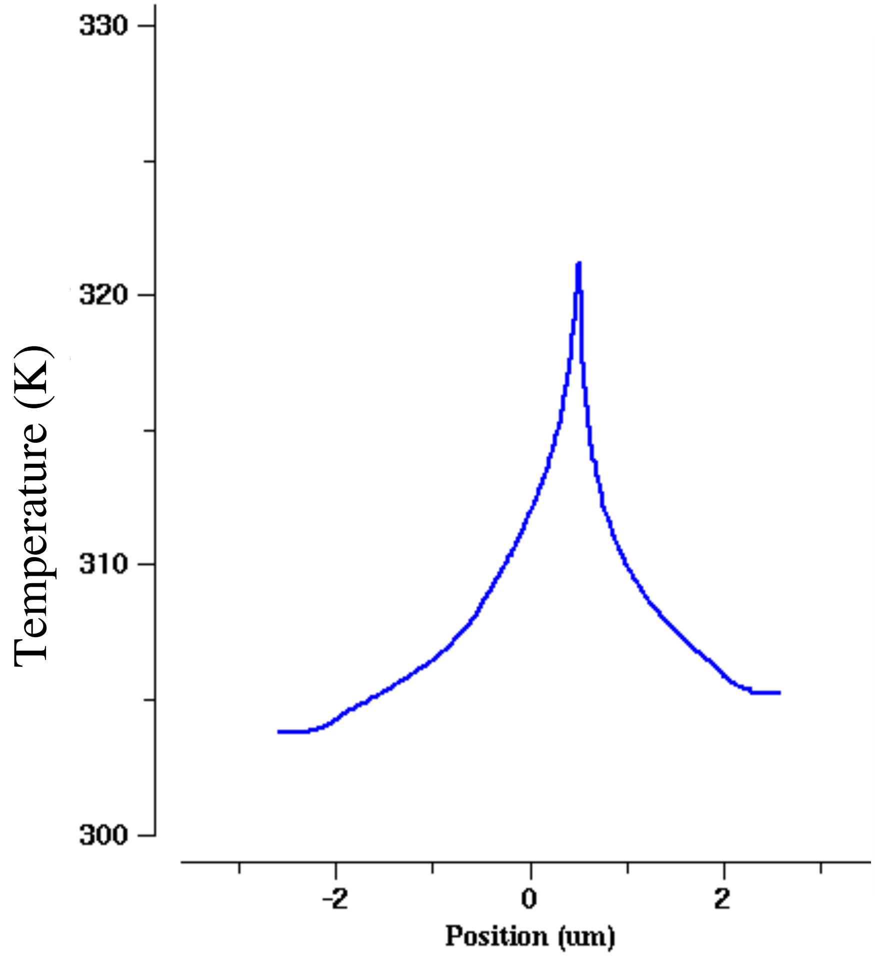
V_G=0 V V_D=8 V

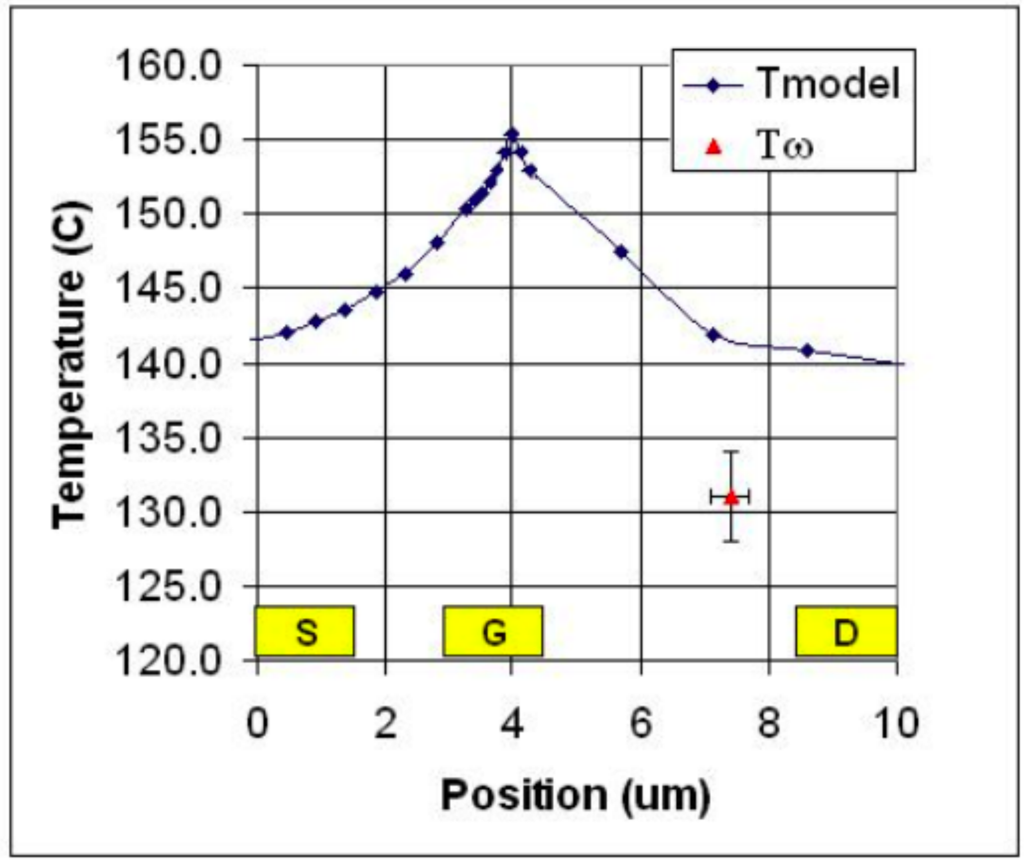


Temperature across device through AlGaN increasing bias

V_G=0 V V_D=0 V to 8 V

Temperature Comparison





Green et. al. Phys. Stat. Sol. (c) **5**, No. 6, (2008)

FLOODS   Power 6.2 W/mm
Baseplate Temp 25 °C

Power 6.2 W   Baseplate Temp 85 °C

Conclusions / Directions

- Bosman, Nishida, Thompson Contributions
- Experimentally Integrated
  - Failure Mechanism Identification feeds M&S
  - Electrical Measurement feeds Model Accuracy

- Direction
  - Integrate Pieces Discussed
  - Connect strain calculations to Temp, Traps
  - Work on Trap Generation - Bosman Connection